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L1 10 ("IN-SOURCE DECAY" OR ISD) AND (CID OR SID OR PID OR LID OR COLLISION? OR "METASTABLE DECAY")

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DOCUMENT NUMBER: 147:206185

TITLE: The disulfide bond pattern of Salmon Egg Lectin 24K from the Chinook salmon *Oncorhynchus tshawytscha*

AUTHOR(S): Yu, Haiqiang; Murata, Kenji; Hedrick, Jerry L.; Almaraz, Ruben T.; Xiang, Fan; Franz, Andreas H.

CORPORATE SOURCE: Department of Chemistry, University of the Pacific, Stockton, CA, 95211, USA

SOURCE: Archives of Biochemistry and Biophysics (2007), 463(1), 1-11

CODEN: ABBIA4; ISSN: 0003-9861

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The disulfide bonds in the galactose-specific lectin SEL 24K from the egg of the Chinook salmon *Oncorhynchus tshawytscha* were determined by mass spectrometry. Four predictive in silico tools were used to determine the oxidation state of cysteines in the sequence and possible location of the disulfide bonds. A combination of tryptic digestion, HPLC separation, and chemical modifications were used to establish the location of seven disulfide bonds and one pair of free cysteines. After proteolysis, peptides containing one or two disulfide bonds were identified by reduction and mass spectral comparison. MALDI mass spectrometry was supported by chemical modification (iodoacetamide) and in silico digestion. The assignments of disulfide bonds were further confirmed by mass spectral fragmentation studies including in-source dissociation (ISD) and collision-induced dissociation (CID). The exptl. determined disulfide bonds and free Cys residues were only partially consistent with those generated by several automated public-domain algorithms.

REFERENCE COUNT: 47

L1 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:314315 CAPLUS <<LOGINID::20070926>>

DOCUMENT NUMBER: 144:483903

TITLE: Matrix-assisted laser desorption/ionization in-source decay combined with tandem time-of-flight mass spectrometry of permethylated oligosaccharides: targeted characterization of specific parts of the glycan structure

AUTHOR(S): Wuhrer, Manfred; Deelder, Andre M.

CORPORATE SOURCE: Biomolecular Mass Spectrometry Unit, Department of Parasitology, Leiden University Medical Center, Leiden, 2300 RC, Neth.

SOURCE: Rapid Communications in Mass Spectrometry (2006), 20(6), 943-951

CODEN: RCMSEF; ISSN: 0951-4198

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Matrix-assisted laser desorption/ionization tandem time-of-flight mass spectrometry (MALDI-TOF/TOF-MS) has been introduced in recent years as a valuable tool for the structural characterization of permethylated oligosaccharides. In this report, the authors describe the combination of MALDI in-source decay (ISD) with the subsequent TOF/TOF-MS analyses of specific fragments, allowing the detailed characterization of the selected part of the oligosaccharide mol. Part of the second-generation fragment ions were different from those observed in conventional MALDI-TOF/TOF-MS expts. Other fragments, which had already been observed in conventional MALDI-TOF/TOF-MS and again showed up in second-generation fragment anal., could be assigned to specific parts of the mol. The authors' approach disclosed different structural features of the oligosaccharides: due to permethylation, the glycosidic linkage fragments allowed the distinction between terminal, monosubstituted and disubstituted monosaccharides and indicated the oligosaccharide sequence. Moreover, substitution positions were deduced based on characteristic cross-ring fragmentation by high-energy collision-induced fragmentation. In conclusion, combination of MALDI-ISD with TOF/TOF-MS allows the detailed characterization of specific moieties of permethylated oligosaccharides and is, therefore, a powerful technique for structural glycomics.

REFERENCE COUNT: 35

L1 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:704798 CAPLUS <<LOGINID::20070926>>

DOCUMENT NUMBER: 141:385846

TITLE: Binding of DNA Purine Sites to Dirhodium Compounds Probed by Mass Spectrometry

AUTHOR(S): Chifotides, Helen T.; Koomen, John M.; Kang, Mijeong; Tichy, Shane E.; Dunbar, Kim R.; Russell, David H.

CORPORATE SOURCE: Chemistry Department and Laboratory for Biological Mass Spectrometry, Texas AM University, College Station, TX, 77843, USA

SOURCE: Inorganic Chemistry (2004), 43(20), 6177-6187

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The adducts formed between the antitumor active compds.

[Rh2(O2CCH3)2(MeCN)6](BF4)2, Rh2(O2CCH3)4, and Rh2(O2CCF3)4 with DNA oligonucleotides were assessed by matrix-assisted laser desorption ionization (MALDI) and nanoelectrospray (nanoESI) coupled to time-of-flight mass spectrometry (TOF MS). MALDI studies performed on dipurine (AA, AG, GA, and GG)-containing single-stranded oligonucleotides of different lengths (tetra- to dodecamers) led to the establishment of the relative reactivity cis-[Pt(NH3)2(OH2)2]2+ (activated cisplatin) » Rh2(O2CCF3)4 > cis-[Pt(NH3)2Cl2] (cisplatin) » [Rh2(O2CCH3)2(MeCN)6](BF4)2 > Rh2(O2CCH3)4 » Pt(C6H6O4)(NH3)2 (carboplatin). The relative reactivity of the

complexes is associated with the lability of the leaving groups. The general trend is that an increase in the length of the oligonucleotide leads to enhanced reactivity for $\text{Rh}_2(\text{O}_2\text{CCH}_3)_2(\text{MeCN})_6(\text{BF}_4)_2$ and $\text{Rh}_2(\text{O}_2\text{CCH}_3)_4$ (except for the case of $\text{Rh}_2(\text{O}_2\text{CCH}_3)_2(\text{MeCN})_6\text{J}^{2+}$, which reacts faster with the GG octamers than with the dodecamers), whereas the reactivity of $\text{Rh}_2(\text{O}_2\text{CCF}_3)_4$ is independent of the oligonucleotide length. When monitored by ESI, the dodecamers containing GG react faster than the resp. AA oligonucleotides in reactions with $\text{Rh}_2(\text{O}_2\text{CCF}_3)_4$ and $\text{Rh}_2(\text{O}_2\text{CCH}_3)_2(\text{MeCN})_6(\text{BF}_4)_2$, whereas AA oligonucleotides react faster with $\text{Rh}_2(\text{O}_2\text{CCH}_3)_4$. The mixed (AG, GA) purine sequences exhibit comparable rates of reactivity with the homopurine (AA, GG) dodecamers in reactions with $\text{Rh}_2(\text{O}_2\text{CCH}_3)_4$. The observation of initial dirhodium-DNA adducts with weak axial (ax) interactions, followed by rearrangement to more stable equatorial (eq) adducts, was achieved by electrospray ionization; the Rh-Rh bond as well as coordinated acetate or MeCN ligands remain intact in these dirhodium-DNA adducts. MALDI in-source decay (ISD), collision-induced dissociation (CID) MS-MS, and enzymic digestion studies followed by MALDI and ESI MS reveal that, in the dirhodium compds. studied, the purine sites of the DNA oligonucleotides interact with the dirhodium core. Ultimately, both MALDI and ESI MS proved to be complementary, valuable tools for probing the identity and stability of dinuclear metal-DNA adducts.

REFERENCE COUNT: 104

L1 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:631207 CAPLUS <<LOGINID::20070926>>

DOCUMENT NUMBER: 141:119795

TITLE: *Determination of terminal sequences via granddaughter spectra from tandem mass spectrometry*

INVENTOR(S): Suckau, Detlev; Resemann, Anja

PATENT ASSIGNEE(S): Bruker Daltonik GmbH, Germany

SOURCE: Ger. Offen., 13 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10301522	A1	20040805	DE 2003-10301522	20030117
GB 2399218	A	20040908	GB 2004-890	20040115
GB 2399218	B	20051228		
US 2004197826	A1	20041007	US 2004-758958	20040116
PRIORITY APPLN. INFO.:			DE 2003-10301522	A 20030117

AB The invention concerns a method for the determination of terminal sequences in biopolymers, especially proteins using a tandem mass spectrometer with ion source for matrix assisted laser desorption in a way that one group of in source decay (ISD) produced ions are subject to further ionization by collisionally-induced decomposition

(CID), surface-induced decomposition (SID), photon-induced dissociation (PID) or laser-induced decay (LID) and the produced granddaughter ions are measured as mass spectra. Tandem-in-space and tandem-in-time mass spectrometer arrangements can be used. Cystine disulfide bridges are split prior mass spectrometric anal. Computer programs are used for spectrum evaluation.

L1 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:337678 CAPLUS <<LOGINID::20070926>>

DOCUMENT NUMBER: 141:332380

TITLE: Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry. A comparison of fragmentation patterns of linear dextran obtained by in-source decay, post-source decay, and collision-induced dissociation and the stability of linear and cyclic glucans studied by in-source decay

AUTHOR(S): Bashir, Sajid; Giannakopoulos, Anastassios E.; Derrick, Peter J.; Critchley, Peter; Bottrill, Andrew; Padley, Henry D.

CORPORATE SOURCE: Institute of Mass Spectrometry, University of Warwick, Coventry, CV4 7AL, UK

SOURCE: European Journal of Mass Spectrometry (2004), 10(1), 109-120

CODEN: EJMSCL; ISSN: 1469-0667

PUBLISHER: IM Publications

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In the first part of this study, fragmentation patterns from a range of dextran oligomers (containing 4-20 anhydro-glucose units) were compared using three different methods of anal. coupled with matrix-assisted laser desorption/ionization (MALDI) mass spectrometry. Collision-induced dissociation (CID), prompt in-source decay (ISD) and post-source decay (PSD) all caused cleavage of the glycosidic bonds. Both CID and, to a lesser extent, ISD caused further cleavage of pyranose rings of the individual sugar residues. There was very little cleavage of pyranose rings detected in the PSD spectrum. Derivatization of the reducing end-groups of the oligo-dextran with 1-phenyl-3-methyl-5-pyrazolone (PMP) restricted cleavage in the MALDI mass spectrometer to the non-reducing end and also enabled the saccharides to be separated by high-performance liquid chromatog. (HPLC) so that a single chain length could be examined as a standard. Maltose was also used as a standard. In the second part of the study, prompt ISD-MALDI mass spectrometry was used to compare the fragmentation of three oligo-glucans, viz. dextran, maltodextrin and α -cyclodextrin, that have different linkages and different secondary structure. The results showed that the degree of fragmentation correlated with the degree of freedom in the saccharide chains in solution as determined by NMR. Dextran, with the most random conformation, was fragmented most whereas there was little evidence of any fragments, not even glycosidic bond breakage, from cyclodextrin, even when the laser power was increased considerably. The fragmentation pattern of maltodextrin was intermediate. The patterns of fragmentation produced by MALDI mass spectrometry, particularly where stds. are available to calibrate the spectrum and the energy of the laser is controlled, can be used to predict the type of linkage present.

REFERENCE COUNT: 30

L1 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:145651 CAPLUS <<LOGINID::20070926>>

DOCUMENT NUMBER: 139:69518

TITLE: The characteristics of in-source decay in mass spectrometric degradation methods -hydrogen-attachment dissociation (HAD)-

AUTHOR(S): Takayama, Mitsuo

CORPORATE SOURCE: Graduate School of Integrated Science, Yokohama City University, Kanazawa-ku, Yokohama, 236-0027, Japan

SOURCE: Journal of the Mass Spectrometry Society of Japan (2002), 50(6), 337-349

CODEN: JMSJEY; ISSN: 1340-8097

PUBLISHER: Nippon Shitsuryo Bunseki Gakkai

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB In-source decay (ISD) combined with matrix-assisted laser desorption/ionization (MALDI) time-of-flight mass spectrometer (TOF MS) has been described by comparing with conventional mass spectrometric degradation (MSD) methods such as collision-induced dissociation (CID) and post-source decay (PSD). The ISD characteristic is the formation of c- and (z+2)-ions originated from the N-Ca bond cleavage on the peptide backbone, while the CID and PSD processes are the CO-NH bond cleavage which brings about b- and y-ion. Furthermore, the ISD processes occurring with 337 nm laser photon irradiation for peptide or protein proceed resulting in the formation of hyper-valent radical species via intermol. hydrogen transfer between matrix and analyte mols. following the non-ergodic N-Ca bond cleavage. The non-ergodic N-Ca bond cleavage occurs in the MALDI ion source within nanosecond order, as an a-cleavage initiated with radical site at the carbonyl carbon. The MALDI-ISD method has been applied to three peptides and five proteins.

L1 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:35684 CAPLUS <<LOGINID::20070926>>

DOCUMENT NUMBER: 138:205551

TITLE: Design of ABC Triblock Copolymers near the ODT with the Random Phase Approximation

AUTHOR(S): Cochran, Eric W.; Morse, David C.; Bates, Frank S.

CORPORATE SOURCE: Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, 55455-0132, USA

SOURCE: Macromolecules (2003), 36(3), 782-792

CODEN: MAMOBX; ISSN: 0024-9297

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Leibler's RPA for block copolymers, modified so as to be applicable to linear multiblock copolymers, has been quant. compared to data from three linear ABC/ACB triblock copolymer melts: poly(cyclohexylethylene-b-ethylene-b-ethylethylene) (CEEE)/CEEE, poly(styrene-b-isoprene-b-ethylene oxide) (SIO)/ISO (Macromols. 2001, 34, 6994-7008; Macromols. 2002, 35, 7007-7017), and poly(styrene-b-isoprene-b-

dimethylsiloxane) (SID)/ISD (Macromols. 2002, 35, 3189-3197). The RPA calcn. provides the mean-field static structure factor for a disordered block copolymer melt, which can be used to anticipate the scattering behavior and spinodal stability limit temperature (Ts); in the context of mean-field theory, the spinodal should lie near the order-disorder-transition temperature (TODT). We find that the RPA spinodal temperature semiquant. matches the magnitude and temperature dependence of the ODT as a function of mol. weight (in CEEE/CEEE) and composition (SIO/ISO). Furthermore, the structure factor also reproduces scattering phenomena in ABC triblock copolymers (ISD/SID) such as the two-peak profile observed in disordered ISD with X-ray scattering. The results show that the RPA is a useful tool in the design of multiblock copolymers without reliance on existing exptl. data or cumbersome numerical SCF calcns.

REFERENCE COUNT: 67

L1 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:173422 CAPLUS <<LOGINID::20070926>>
DOCUMENT NUMBER: 136:341251
TITLE: Model ABC Triblock Copolymers and Blends near the Order-Disorder Transition
AUTHOR(S): Hardy, Cordell M.; Bates, Frank S.; Kim, Man-Ho; Wignall, George D.
CORPORATE SOURCE: Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Macromolecules (2002), 35(8), 3189-3197
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We report differences in the thermodyn. behavior of compositionally sym. ABC and BAC triblock copolymers near the order-disorder transition temperature and of binary ABC/BAC copolymer blends: poly(styrene-b-isoprene-b-dimethylsiloxane) (SID) and ISD with segment volume fractions near 0.33 and similar mol. weight disorder at different temps. and from different ordered-state symmetries. Blends of sym. SID and ISD mols. with mol. wts. near 10 K are miscible and form a gyroid morphol. over a wide range of blend compns. Flory-Huggins interaction parameters for this ABC system allow a detailed interpretation of SAXS, SANS, and DMS measurements. Sym. SID disorders from the lamellar state, while ISD disorders from hexagonally packed cylinders of D blocks in a mixed matrix of S and I blocks. Block mixing occurs to reduce the number of S-D interactions forced by chemical connectivity in ISD. This drive to minimize unfavorable interactions is the underlying cause of the results outlined in this report.

REFERENCE COUNT: 46